Reviewer Report

Title: Tool recommender system in Galaxy using deep learning

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Reviewer name: Jeremy Leipzig

Reviewer Comments to Author:

The authors present a Galaxy tool recommendation system based on a training set of over 200,000 tool sequences from existing workflows. The final version of this system uses a GRU neural network.
Although extensive testing was done to compare and benchmark this model with other neural networks, it should be noted there is no existing conventional approach (Markov Model/market basket/Bayesian) but I don't feel that it is necessary to create a straw man for this purpose. The neural network offers a high degree of accuracy without the need to manually annotate each tool.
The description of the GRU implementation, testing, and optimization is very good and will inform readers about how to implement similar solutions for other applications. The Github repository is also well organized. This paper is well suited to this journal and should be accepted with minor revisions.
I have three minor revisions to suggest:
1. I think most readers would understand what overfitting would look like in a typical machine learning, but maybe not in a recommendation engine for tools. What noise or error that is propagated by an overfit recommendation engine? For instance, would it resemble obscure tools that some edge case user chose? More importantly, what does the regularization step actually do in this case - recommend a repertoire of more common tools, or simply remain agnostic?
Provide a real-world example, something like…
"An example of overfitting in our recommendation system may involve tools with few use cases (e.g. tools for dealing with organisms with no reference assembly). The GRU would learn only from a limited training set and which could recommend tools that would not be appropriate for most users."
2. It appears the recommendation engine cannot recommend entirely new tools without completely rebuilding the model. Please explain how often the model is rebuilt in practice. Also explain how new tools would ever be recommended if they don't appear in existing workflows. Is the design that entirely new tools would be adopted into workflows by "power users" and therefore trickle down to more casual Galaxy users?
3. DESeq2 is miscapitalized as DeSeq2 on pg2

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